OSCARS
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FAIRMD

Disorder to Order: Streamlining Biomolecule Simulation Re-Use with FAIR NMRlipids Database

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Implemented by

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CHALLENGE ADDRESSED

There is no central "PDB-like" structural databank for disordered biomolecules

-> Barrier, e.g., for AI-driven research

For membrane lipids there is the open NMRlipids Databank

-> Aim: Help understanding cellular membranes

-> Contains Molecular Dynamics (MD) simulation trajectories

-> Trajectories quality-evaluated against experimental data

-> Little interoperability with other databanks

No similar databank for intrinsically disordered proteins (IDPs)

-> Even though IDPs are crucial: found in 30% of eukaryotic proteome

FAIRMD expands the NMRlipids Databank to disordered proteins

-> MD simulation trajectories of IDPs

-> “overlay” databank structure, as for lipids

-> Quality-evaluation against NMR relaxation rates, SAXS, and PRE

-> API access

In addition, it expands the interoperability of NMRlipids Databank

-> Annotation with existing PID: InChlKeys, SMILES, Swisslipids IDs

-> Implementing Bioschema to increase findability

-> Crosslinking with LIPIDMAPS, SwissLipids, DisProt

RESULTS

IDP-expanded NMRlipids Databank enables

-> Analysis of lipid and IDP structural properties at atomistic detail

-> Analysis of dynamical properties from picoseconds to hundreds of nanoseconds

-> Development of coarse grained or AI models to predict such properties

Better findability and interoperability of NMRlipids Databank enables

-> Enhanced open collaboration in Biomolecular simulations

-> Solving practical challenges in data distribution with overlay databanks

RISKS

Lack of community uptake

-> Gauge IDP community needs by approaching key players

-> Organize community engagement events

Difficulties of maintaining implementation

-> Build on existing frameworks

Defining a reliable and understandable IDP simulation quality measure

-> Engage the community in open discussion

Using the NMRlipids “brand” in the IDP context

-> Make FAIRMD the main “brand” with sub-brands

TEAM

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